Computer Models of Nonwoven Geometry and Filtration Simulation

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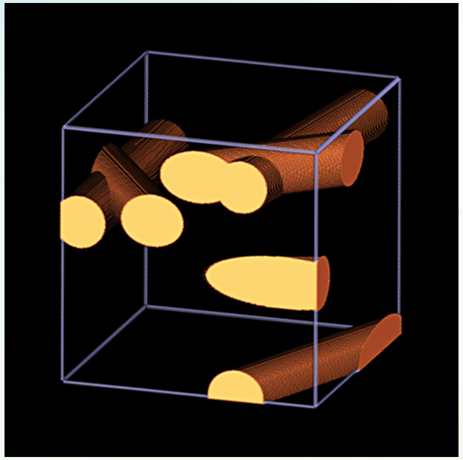
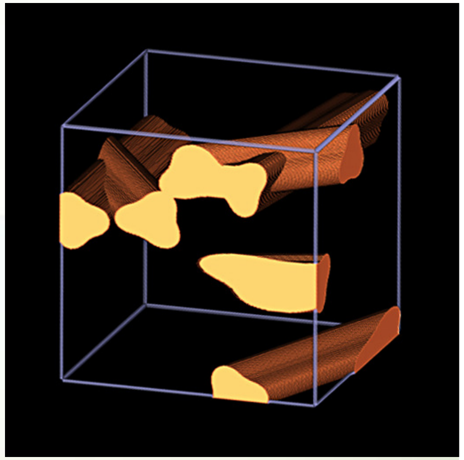
Part I: 3d Nonwoven Model

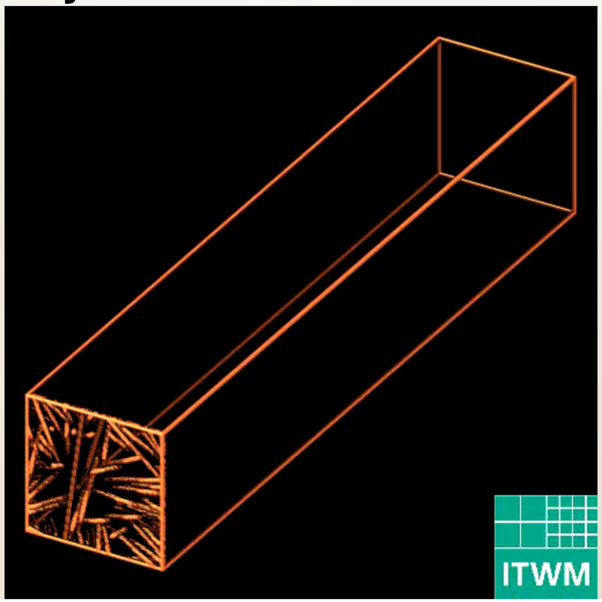
- Fiber diameter, length
- Fiber shapes
- Fiber directions
- Fiber crimp, overlap
- Porosity
- # of Layers, thicknesses

Shape

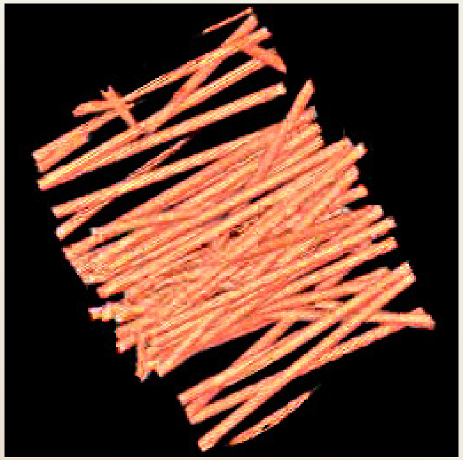




Layers

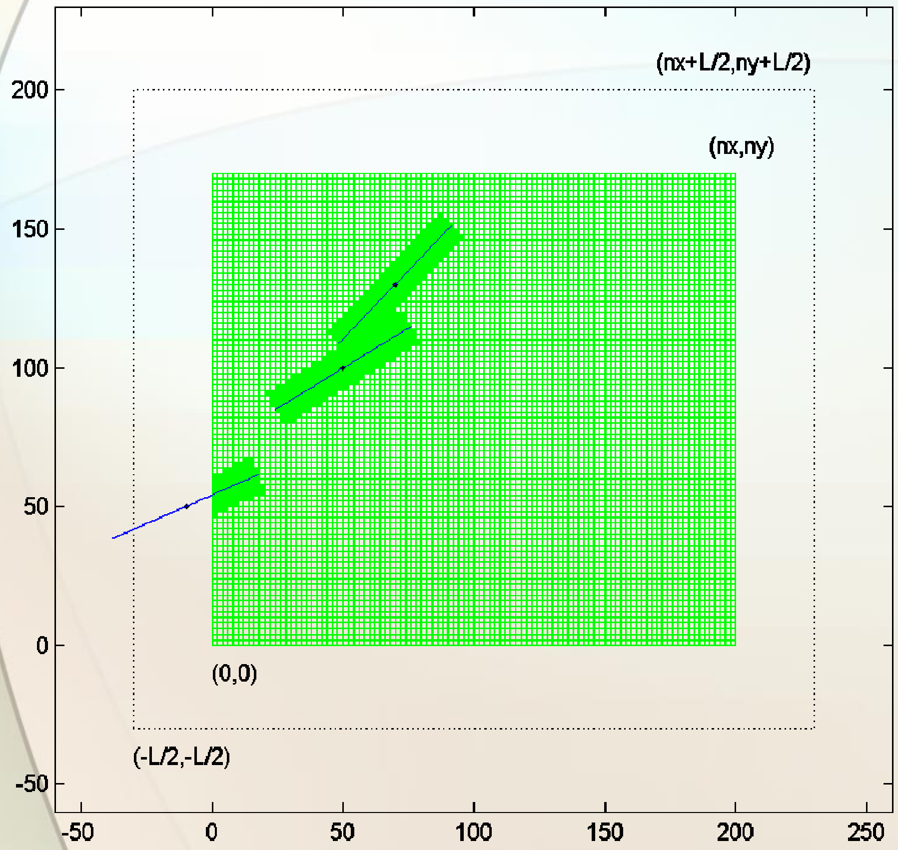


Directions



Diameters

Model parameters and realization



"Manufacturable" parameters:

- Porosity
- Fiber diameter & length (distributions)
- Fiber orientation distribution

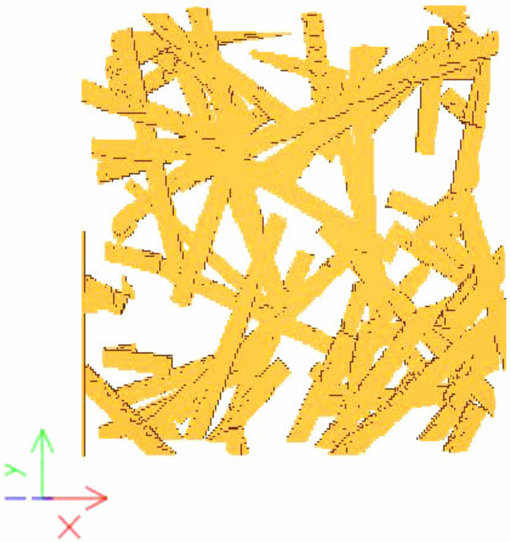
Generator:

- Choice of uniform Cartesian REV
- Random center point location
- Random fiber orientation
- Discretization via distance from axis
- Until desired porosity is reached

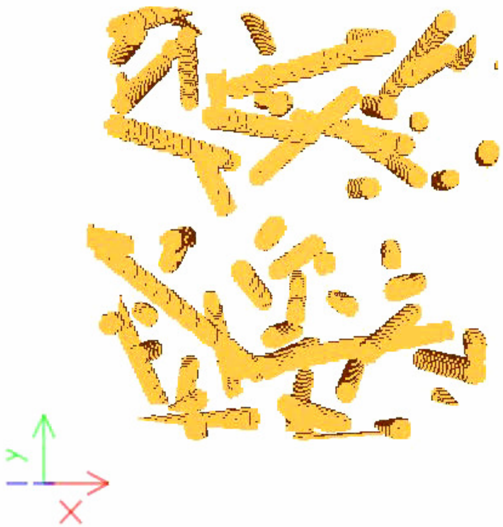
Extra effects:

- Partly exterior fibers
- Overlapping fibers

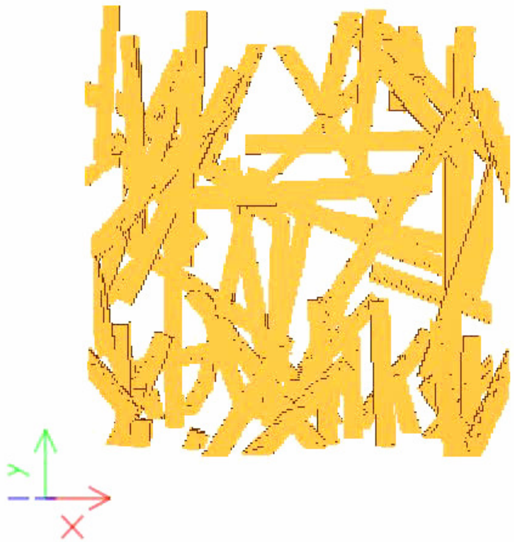
Geometric meaning of anisotropy



Planar isotropy

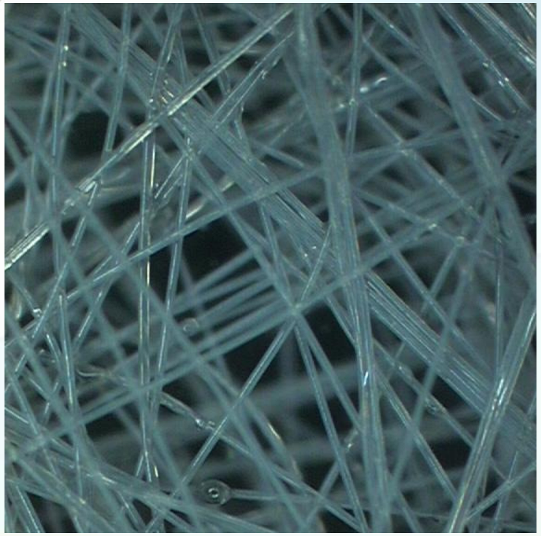


Parallel

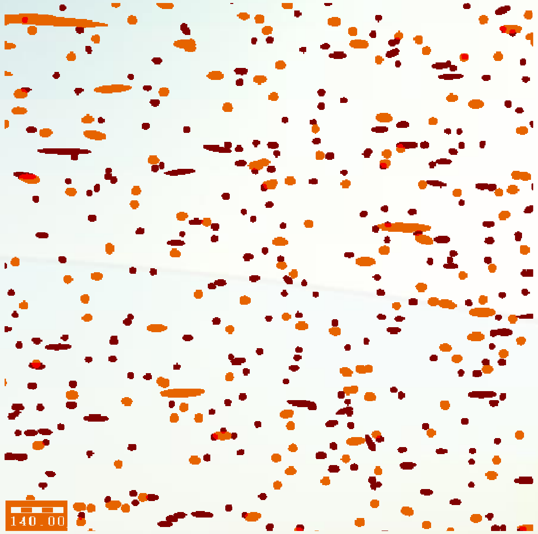


2-fold anisotropy

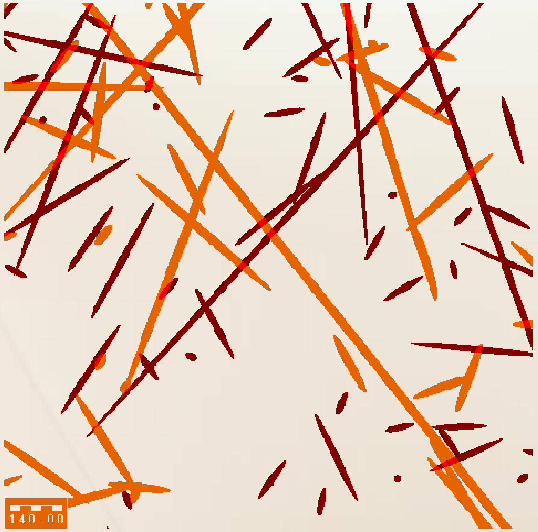
Real and generated nonwoven



Microscopy (real)



ZY-cross section

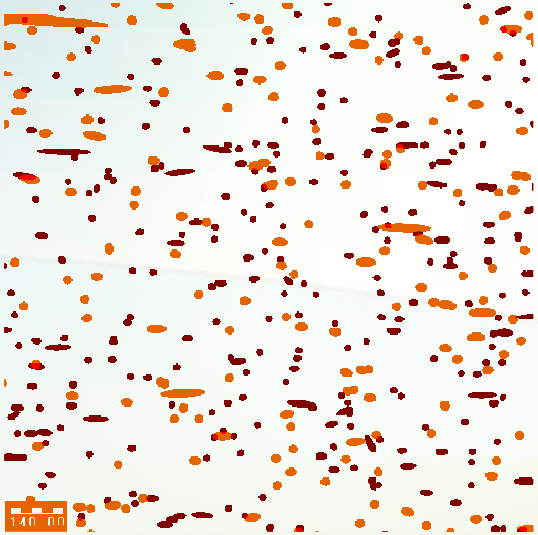


XY-cross section

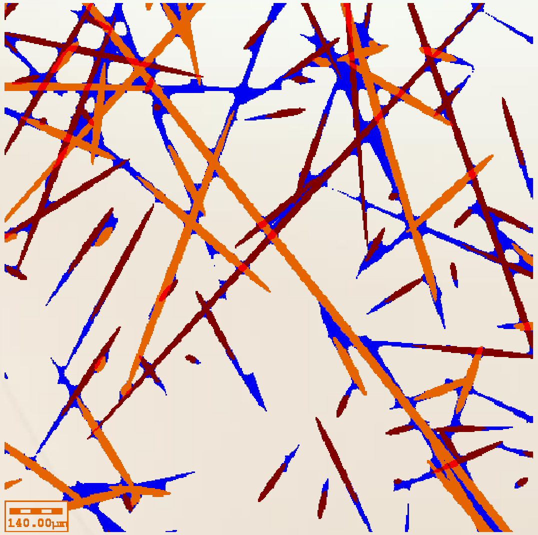
3D view

Nonwoven with binder; under compression

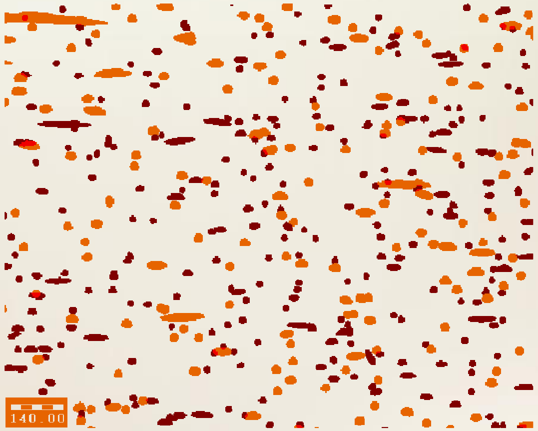
XY-cross section



ZY-cross section

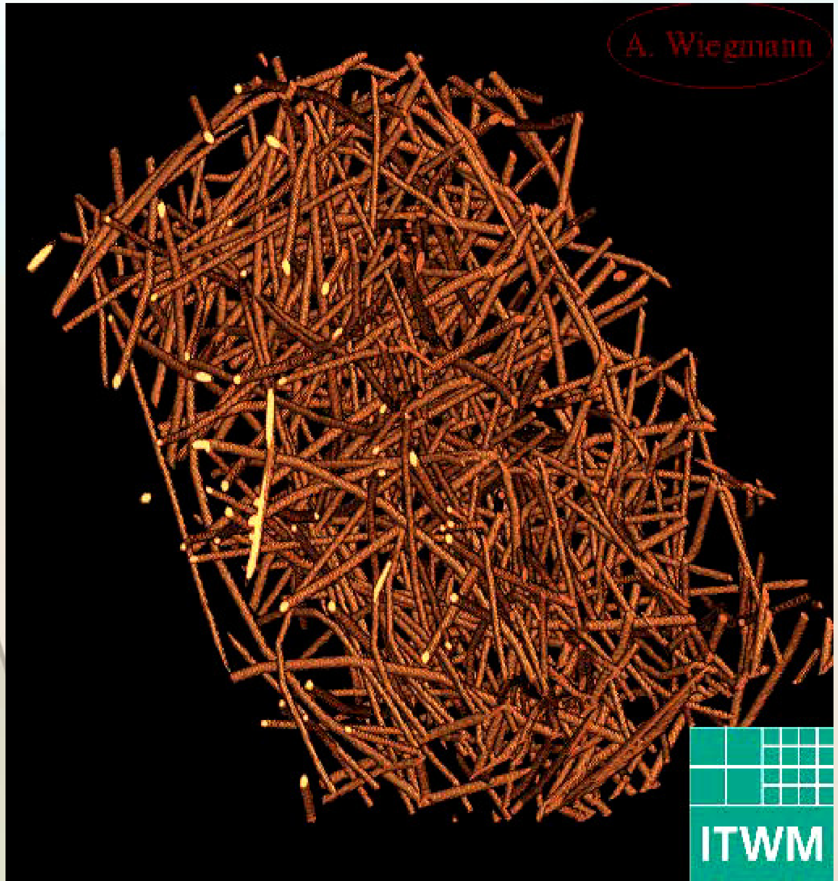


XY-cross section,
with binder



ZY-cross section,
compressed

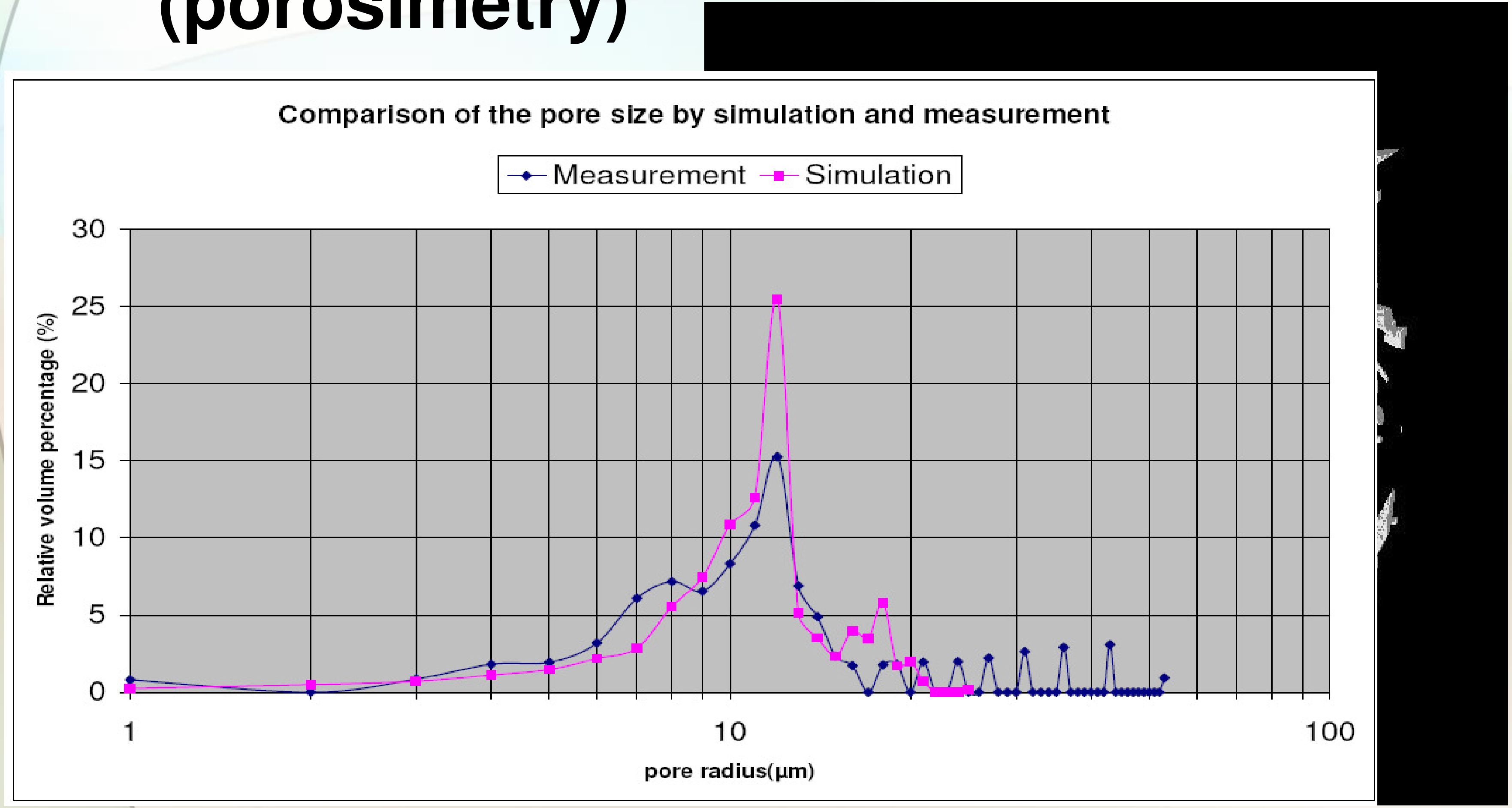
Compression for oil filtration



- Currently purely geometric
- Must still be connected to the oil pressure

Model validation

- Simulated and real nonwoven
- Simulated and real mercury intrusion (porosimetry)



Part II: Flow through Nonwoven

$$-\mu\Delta\vec{u} + \nabla\vec{u}\cdot\vec{u} + \kappa^{-1}\vec{u} + \nabla p \;=\; \vec{f} \text{ (momentum balance)}$$

$\vec{f}$

We do NOT use Fluent, but

- A proprietary Lattice Boltzmann code *Parpac*
- A proprietary Finite Volume code *EJ-Stokes*

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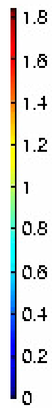
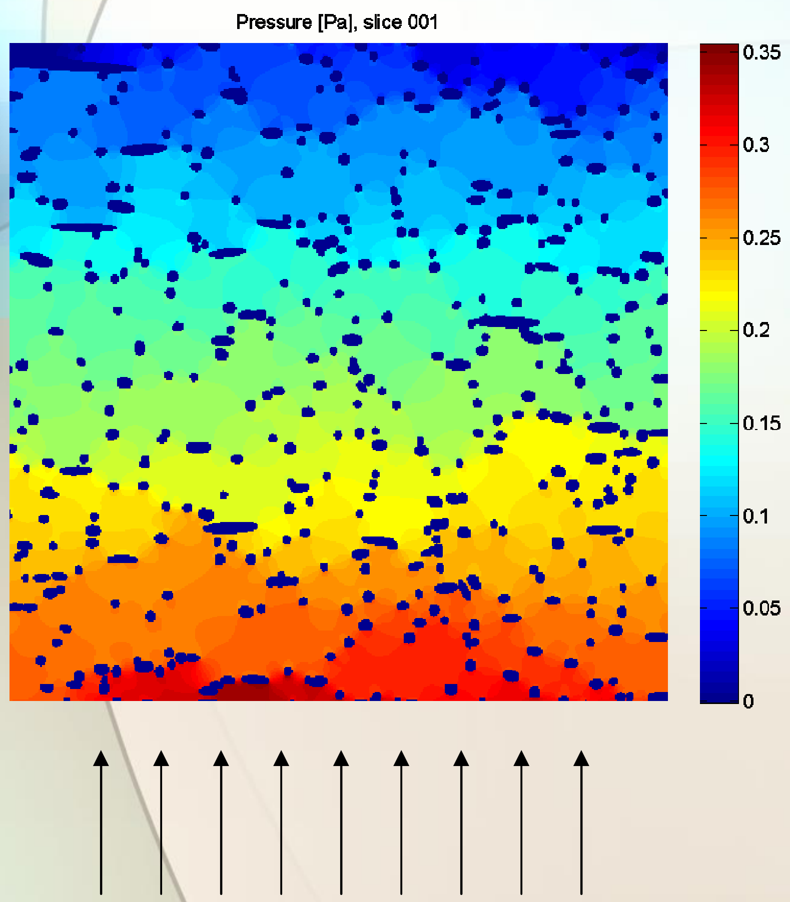
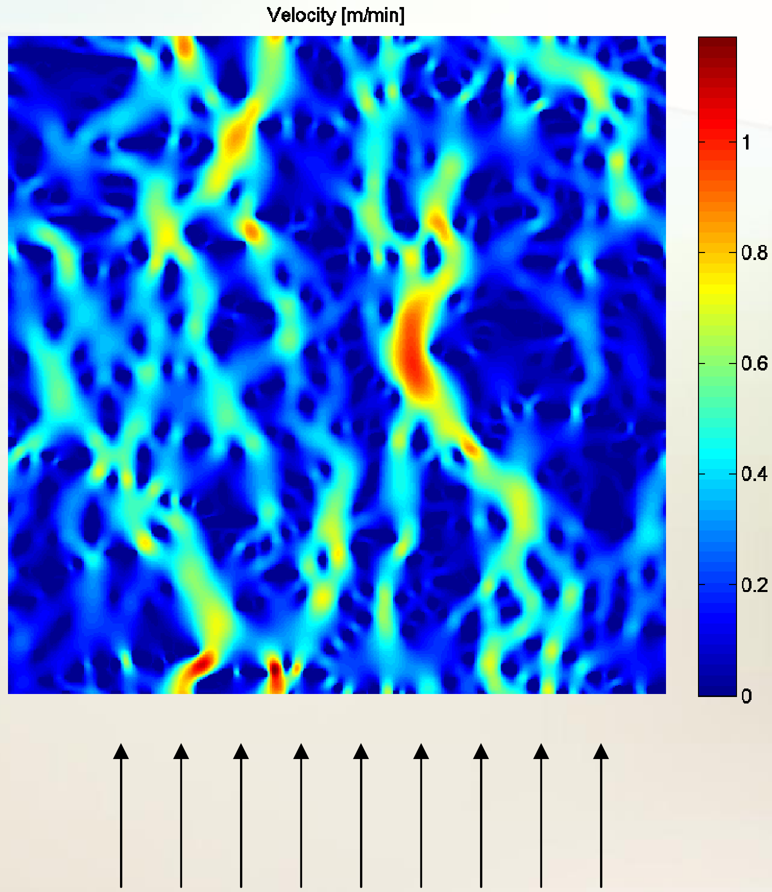


Pressure and velocity

Pressure (p)



Velocity ($\vec{u}$)



Permeability from Stokes equations

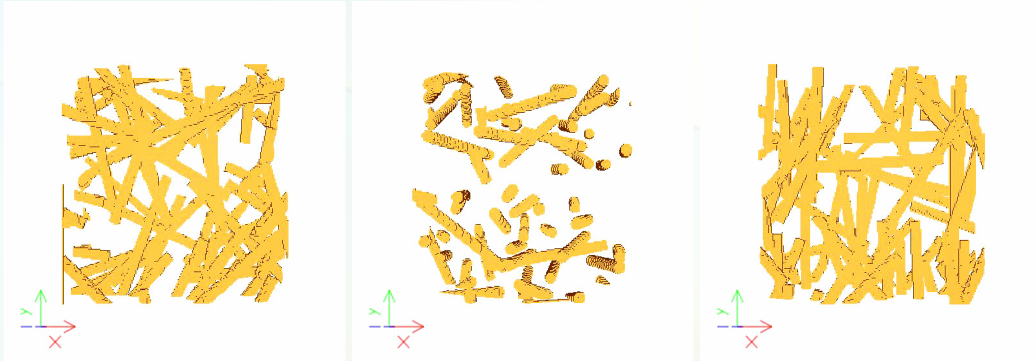
Mean velocity from nano simulation: $\bar{\mathbf{u}}_i$ is mean value of solution of a periodic Stokes problem

$$
\begin{aligned}
\nabla \cdot \mathbf{u}_i &= 0 \text{ (mass conservation)},\\
\mathbf{u}_i &= 0 \text{ on } \Gamma \text{ (no-slip on solid surfaces)},\\
-\mu \Delta \mathbf{u}_i + \nabla p &= \begin{pmatrix} \delta_{i1} \\ \delta_{i2} \\ \delta_{i3} \end{pmatrix}.
\end{aligned}
$$

Then make Darcy-Ansatz $\bar{\mathbf{u}}_i = -\frac{\kappa}{\mu} \begin{pmatrix} -\delta_{i1} \\ -\delta_{i2} \\ -\delta_{i3} \end{pmatrix}$ and get

$$
\begin{aligned}
\kappa_{*1} &= \mu \bar{\mathbf{u}}_1,\\
\kappa_{*2} &= \mu \bar{\mathbf{u}}_2,\\
\kappa_{*3} &= \mu \bar{\mathbf{u}}_3.
\end{aligned}
$$

Permeability (in 1e-011m^2)

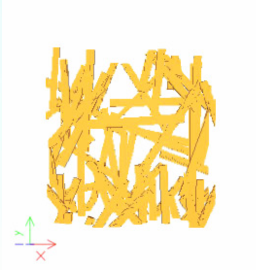


103.00	5.28	-2.81	81.50	2.64	-5.05	92.90	0.873	-0.153
5.29	108.00	-1.55	2.67	79.10	0.142	-0.848	120.00	-3.75
-2.81	-1.55	79.90	-5.07	0.150	124.00	-0.152	-3.75	80.30

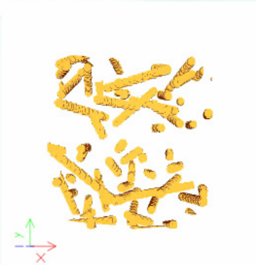
- Computations require ca. 17 iterations or 5 minutes per column (45 minutes for all 3 tables) for 2 digits on 160^3 data sets on my 512 MB laptop
- Geometric anisotropy in Cartesian directions results in almost diagonal & symmetric (up to precision) tensor

Permeability (in 1e-011m^2)

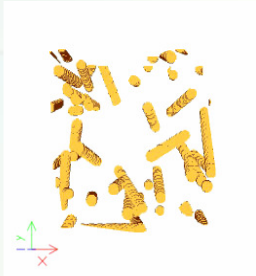
κ_{11} = 93 β_1 = 10
κ_{22} = 120 β_2 = 3
κ_{33} = 80 ρ = 5%
d = 8µm



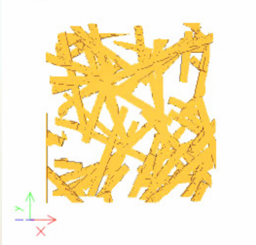
κ_{11} = 82 β_1 = 0.1
κ_{22} = 79 β_2 = 1
κ_{33} = 124 ρ = 5%
d = 8µm



κ_{11} = 104 β_1 = 10
κ_{22} = 121 β_2 = 1
κ_{33} = 195 ρ = 5%
d = 10µm

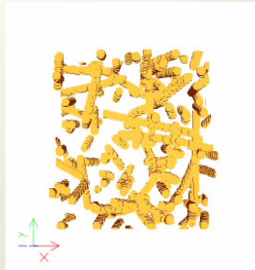


κ_{11} = 103 β_1 = 10
κ_{22} = 108 β_2 = 1
κ_{33} = 80 ρ = 5%
d = 8µm



κ_{11} = 40 β_1 = 10
κ_{22} = 40 β_2 = 1
κ_{33} = 67 ρ = 7%
d = 8µm

κ_{11} = 28 β_1 = 10
κ_{22} = 29 β_2 = 1
κ_{33} = 48 ρ = 9%
d = 8µm



κ_{11} = 55 β_1 = 10
κ_{22} = 48 β_2 = 1
κ_{33} = 87 ρ = 5%
d = 6µm

Expect now at most 10% deviation of mean values compared with measurements for nonwoven

Part III: Particle Motion & Filtration

$$
\begin{aligned}
d\vec{v} &= -\gamma \times (\vec{v}(\vec{x}) - \vec{v}_\circ(\vec{x}))\, dt + \frac{Q\vec{E}_\circ(\vec{x})}{m} dt + \sigma \times d\vec{W}(t) \\
\frac{d\vec{x}}{dt} &= \vec{v} \\
\gamma &= 6\pi\rho\mu\frac{R}{m} \\
\sigma^2 &= \frac{2k_B T\gamma}{m} \\
\left\langle dW_i(t), dW_j(t) \right\rangle &= \delta_{ij} dt
\end{aligned}
$$

Friction with fluid — Electric attraction — Diffusive motion

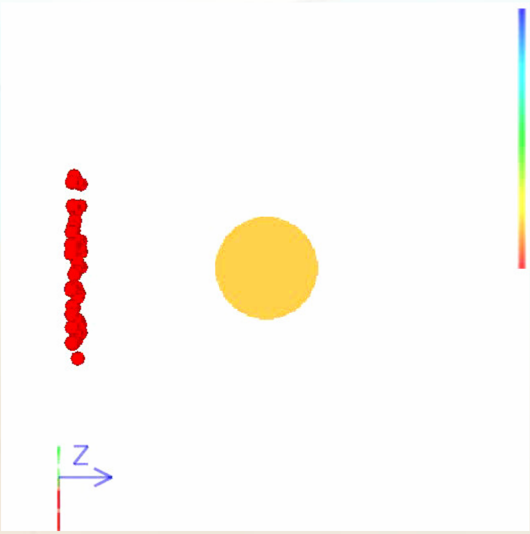
t:	time
$\vec{x}$:	particle position
$\vec{v}$:	particle velocity
R:	particle radius
m:	particle mass
Q:	particle charge
T:	ambient temperature
k_B:	Boltzmann constant
):	3d probability (Wiener) measure
	electric field
	fluid velocity
	fluid density
	fluid viscosity

Description applies to:

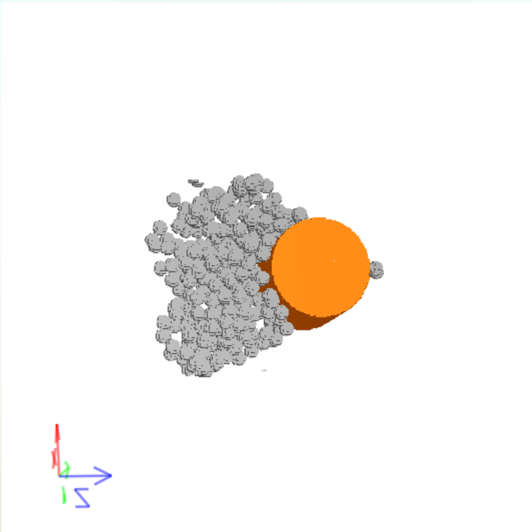
- Oil filtration
- Air filtration
- [Aerosol filtration]

Influence of electric charge (air filtration)

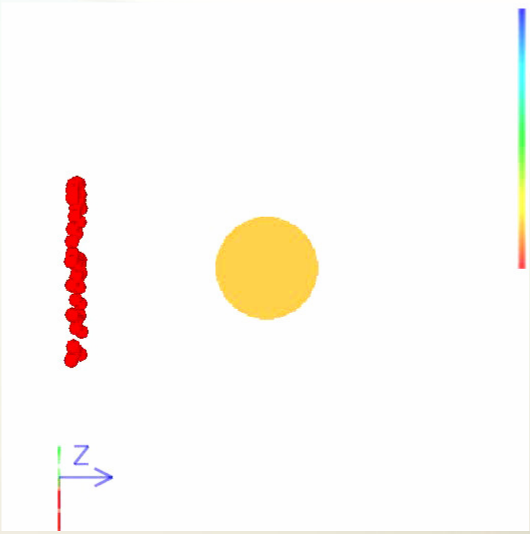
No charges



Low charges

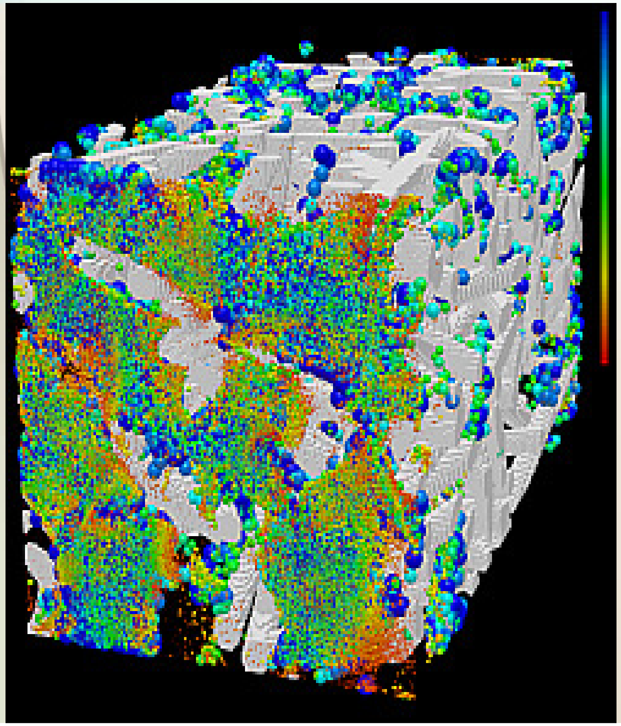


High charges

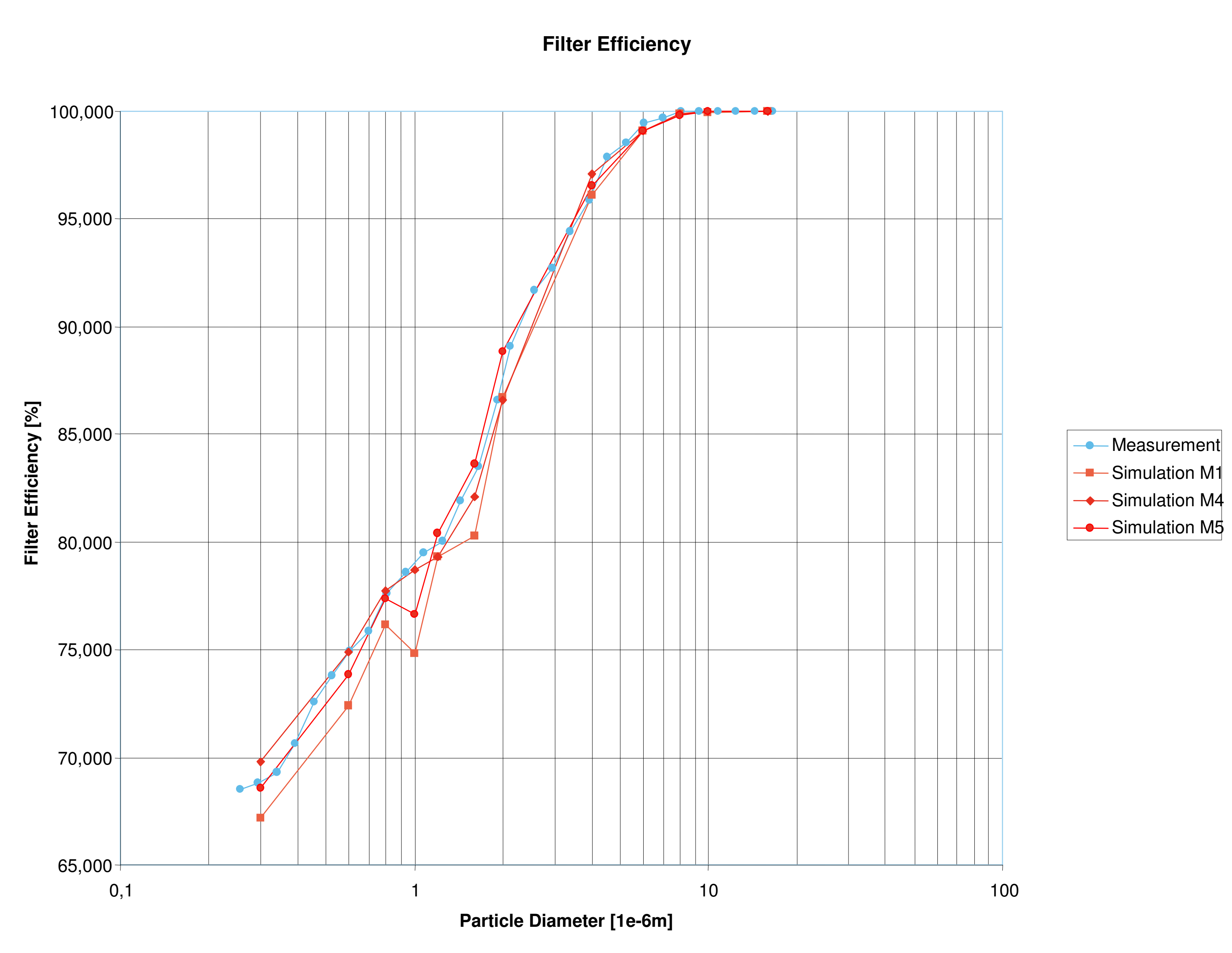


Snapshot of small & large particles

- Particles at fixed travel time, do not interact
- Blue: largest
- Green
- Yellow
- Red: smallest

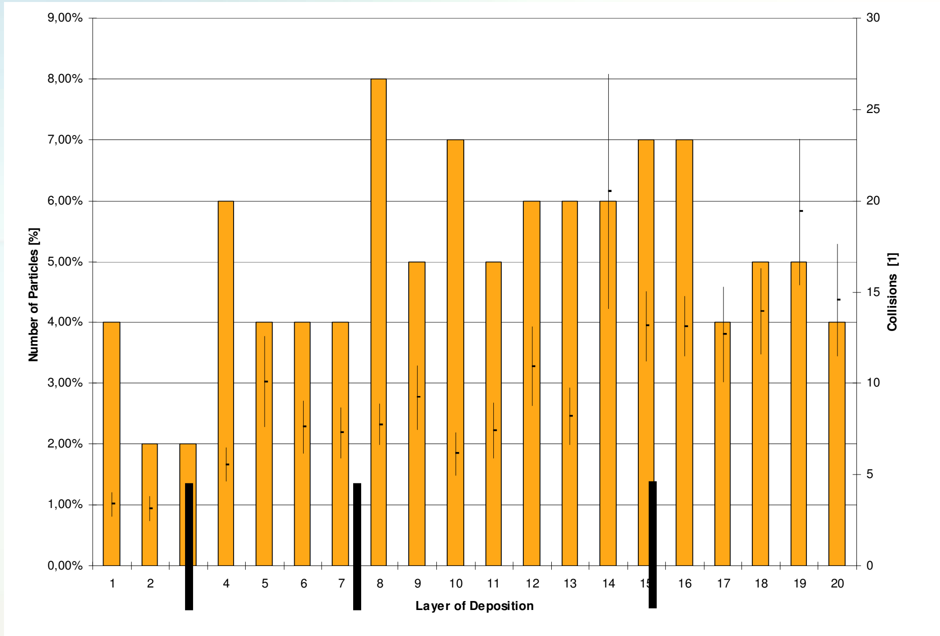


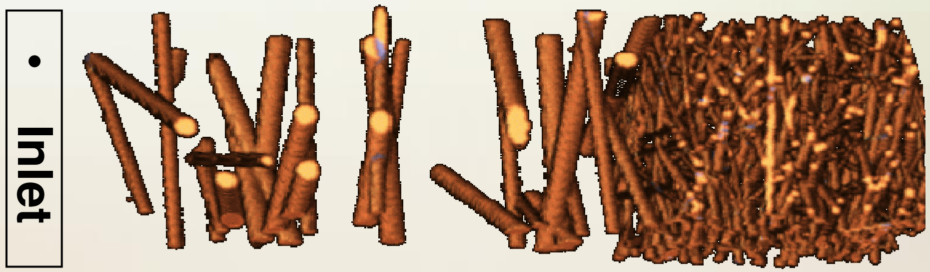
Filter efficiency, measured & simulated



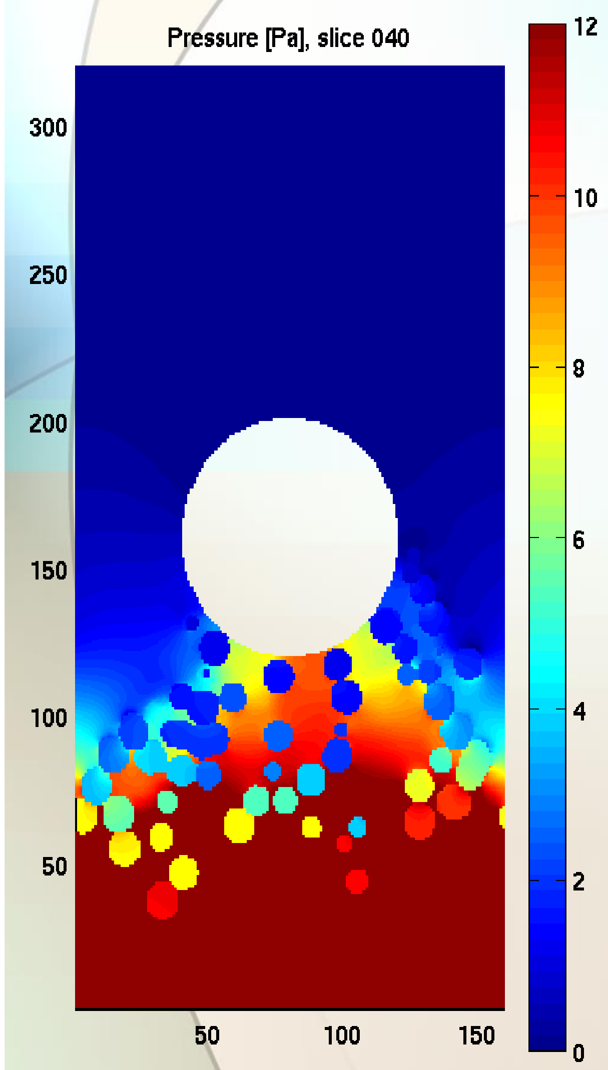
Deposition Diagram

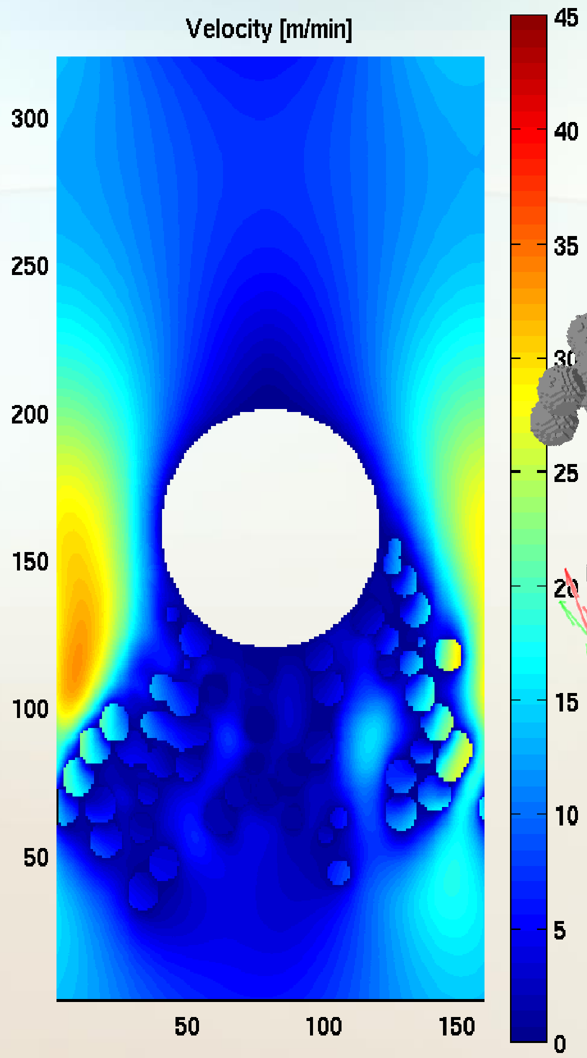
- Deposition locations are 20 64µm layers.
- Orange: particle numbers
- Lines: mean value and standard deviation of number of collisions
- Example: Layer 15 contains 7% of the filtered particles. Those had on average 13.15 collisions with standard deviation 1.9
- 4 layers of gradient material indicated by thick black lines: |

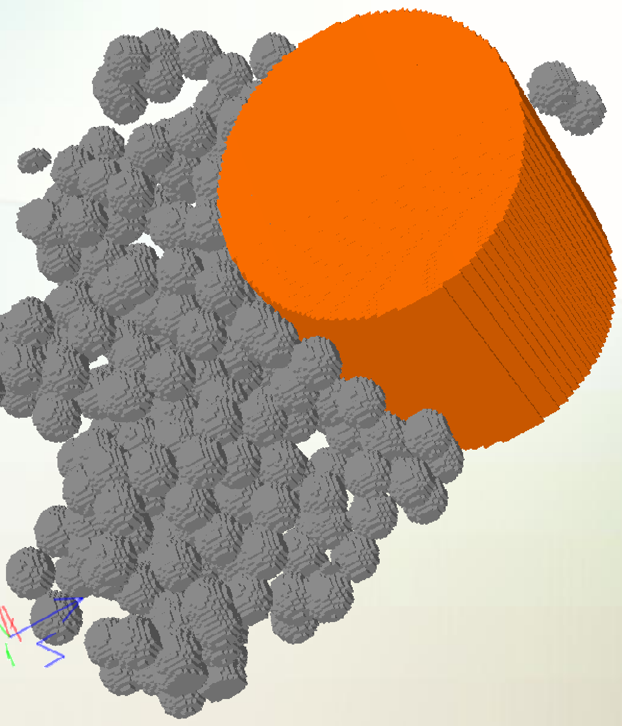




Pressure & velocity in clogging simulation

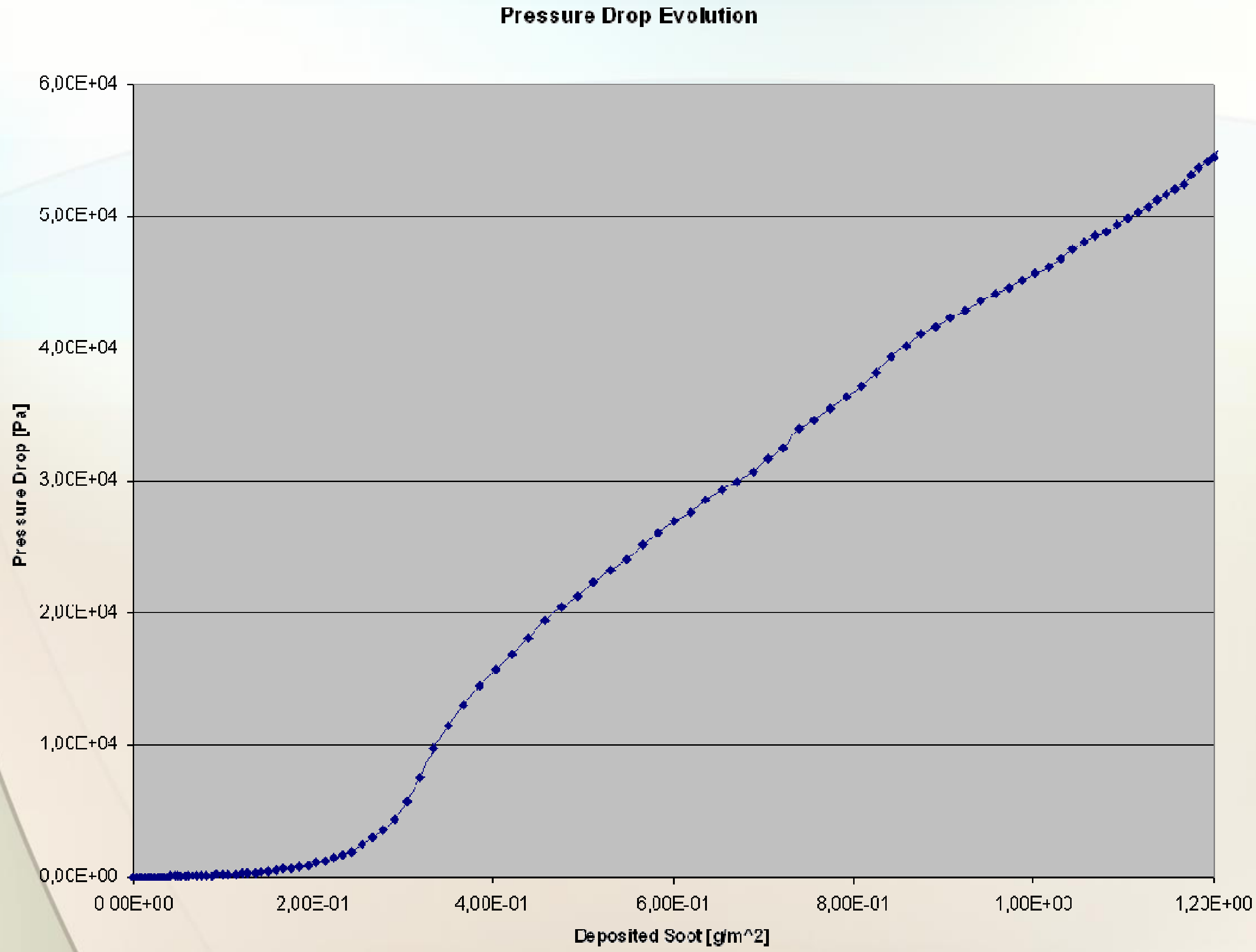






Evolution of pressure drop

- Pressure drop over time or amount



Particle filtration: soot, oil, blood, air, …

Solve ca. 500^3 Stokes flow problems in hours. Unfortunately, in filtration applications must iterate this over many geometries.

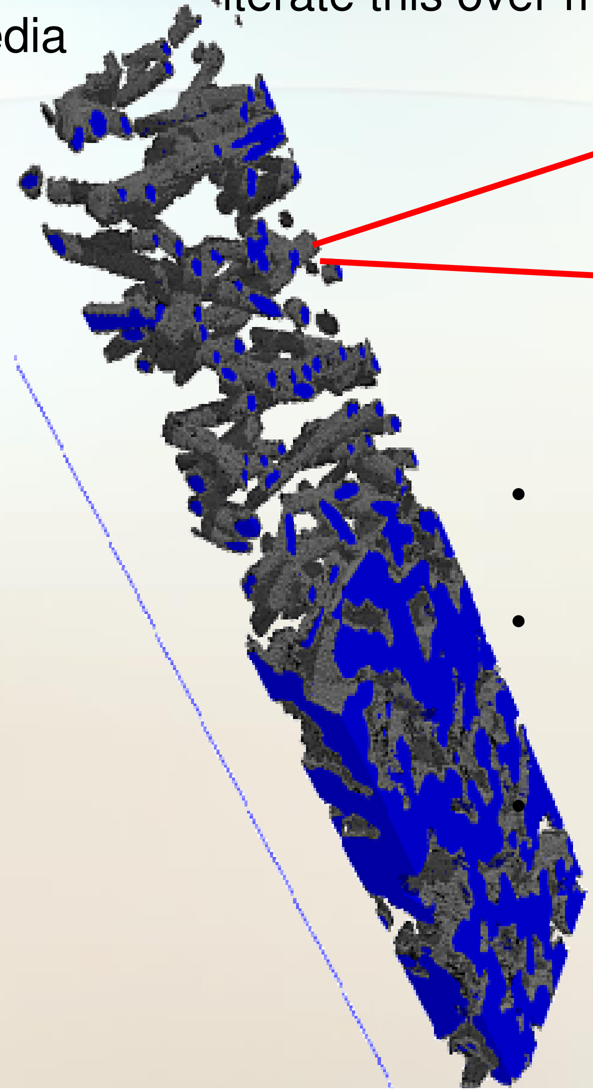
Optimization of

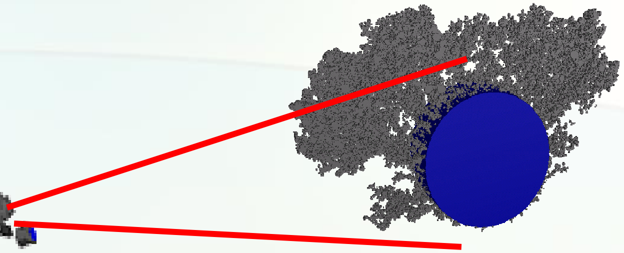
- Filter efficiency of filter media
- Pressure drop
- Life time
- Manufacturing cost

Treatment of

- „intelligence“
- deformation

of white blood cells





Deposition in filter media, with porous voxels, 2d and 3d

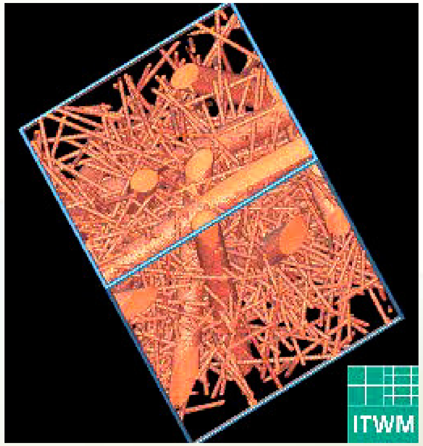
- Soot deposition on single fiber, resolved
- Computation of soot cake on fiber, derive permeability of cake
- Computation of time-dependent clogging of filter media.

The Virtual Filter Material Design Cycle

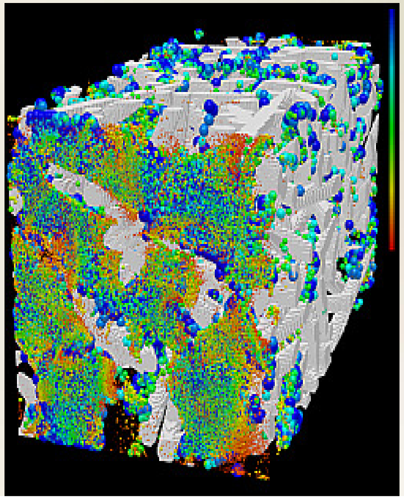
1. Identify parameters for real, existing material
2. Generate volume image for parameters
3. [Solve electric potential]
4. Solve Stokes(-Brinkmann) equations
5. Solve particle motion & deposition
6. Compute filter efficiency, pressure drop/ filter life time
7. Modify material parameters

REM

Generated



Clogged nonwoven



Summary

- I: Nonwoven model
  - Porosity, Fiber direction, Fiber shape
  - Random, voxelized
- II: Flow through Nonwoven
  - Stokes equations, Permeability (= flow resistivity, = flow rate)
- III: Filtration
  - Brownian motion, friction w. fluid
  - Particle size distribution
  - Particle deposition, clogging
  - Pressure drop, efficiency, life time

Find out more:

GeoDict

www.geodict.com

FilterDict

Thank you for attending this presentation.